

The following methods may be used for determining the regularization parameters of the operator R:

- a) the discrepancy principle with a pre-estimate of the variance of measurement errors in the data as described by Tikhonov et al. In 1995;
- b) the method of the L-curve as described by Hansen & O'Leary in 1991;
- c) the method of additional set of calibration data as described by Szczeciński et al. in 1995.

Calibration is also described above with relation to an exemplary embodiment thereof.

Optionally, the isolated peak $v_s(\lambda, l)$ is assumed to have the following forms:

- a) the Dirac distribution $\delta(\lambda)$ for all values of l ;
- b) a triangle whose width is constant or varying versus l ;
- c) a rectangle whose width is constant or varying versus l ;
- d) a Gauss function whose width is constant or varying versus l ; and,
- e) a Lorenz function whose width is constant or varying versus l .

Optionally, at least one of the following methods is used for estimation of the apparatus function $g(\lambda)$:

- a) smoothing approximation applied directly to the data $\{\tilde{y}_n^{cal}\}$ if the isolated peak $v_s(\lambda, l)$ is assumed to have the form of the Dirac distribution $\delta(\lambda)$;
- b) deconvolution of the data $\{\tilde{y}_n^{cal}\}$ with respect to $s(\lambda; l^{cal}, a^{cal})$; and
- c) subsequent use of deconvolution and smoothing approximation.

Optionally, at least one of the following methods may be used for determining other parameters of the operator R:

- a) a direct transformation of the parameters of the operator G;
- b) the minimization of any norm of the solution $\|p_R\|$ under constraints imposed on another norm of the discrepancy $\|s(\lambda; l^{cal}, a^{cal}) - R[\{\tilde{y}_n^{cal}\}; p_R]\|$;
- c) the minimization of any norm of the discrepancy $\|s(\lambda; l^{cal}, a^{cal}) - R[\{\tilde{y}_n^{cal}\}; p_R]\|$ under constraints imposed on another norm of the solution $\|p_R\|$.

Optionally, at least one of the following methods is used for estimation of magnitudes a of peaks, given the estimates \hat{l} of their positions l :

$$\hat{a} = \arg_{a \in A} \inf \{ \|\{\tilde{y}_n\} - G[s(\lambda; \hat{l}, a); p_G]\|_q | a \in A \};$$

and

$$\hat{a} = \arg_{a \in A} \inf \{ \|s(\lambda) - s(\lambda; \hat{l}, a)\|_q | a \in A \}$$

with A —being a set of feasible solutions; options: $q=2$ and $A \subset \mathbb{R}^k$; $q=\infty$ and $A \subset \mathbb{R}^k$; $q=2$ and $A \subset \mathbb{R}_+^k$; $q=\infty$ and $A \subset \mathbb{R}_+^k$. Some examples of algorithmic solutions are given in Deming S. N., Morgan S. L.: *Experimental Design: A Chemometric Approach*, Elsevier 1987; Fraser R. D. B., Suzuki E.: "Biological Applications". In: *Spectral Analysis—Methods and Techniques* (ed by J. A. Balckburn), M. Dekker, 1970, pp. 171–211; Fister III J. C., Harris J. M.: "Multidimensional Least Squares Resolution of Excited State Raman Spectra", *Anal. Chem.*, Vol. 67, No. 4, 1995b, pp. 701–709; Fister III J. C., Harris J. M.: "Multidimensional Least Squares Resolution of Raman Spectra from Intermediates in Photochemical Reactions", *Anal. Chem.*, Vol. 67, No. 8, 1995a, pp. 1361–1370; Goodman K. J., Brenna T.: "Curve Fitting for Restoration of Accuracy of Overlapping Peaks in Gas

Chromatography/Combustion Ratio Mass Spectrometry", *Anal. Chem.*, Vol. 66, No. 8, 1994, pp. 1294–1301; Miekina et al., "Incorporation of the Positivity Constraint into a Tikhonov-method-based Algorithm of Measurand Reconstruction". *Proc. IMEKO-TC1&TC7 Colloquium (London, UK, Sep. 8–10, 1993)*, pp. 299–304 and so forth. A particularly effective solution of the above optimization problem is based on a non-stationary Kalman filter or an adaptive LMS algorithm as described in Ben Slima M., Szczeciński L., Massicotte D., Morawski R. Z., Barwicz A.: "Algorithmic Specification of a Specialized Processor for Spectrometric Applications", *Proc. IEEE Instrum. & Meas. Technology Conf. (Ottawa, Canada, May 19–21, 1997)*, pp. 90–95 and in Ben Slima M., Morawski R. Z., Barwicz A.: "Kalman-filter-based Algorithms of Spectrophotometric Data Correction—Part II: Use of Splines for Approximation of Spectra", *IEEE Trans. Instrum. & Meas.*, Vol. 46, No. 3, June 1997, pp. 685–689.

Optionally, methods for estimation of the magnitudes a are used for iterative correction of estimates of magnitudes a and positions l of the peaks. Known methods include the following:

$$\hat{l} = \arg_{l \in L} \inf \{ \|\{\tilde{y}_n\} - G[s(\lambda; l, \hat{a}); p_G]\|_q | l \in L \}$$

and,

$$\hat{l} = \arg_{l \in L} \inf \{ \|s(\lambda) - s(\lambda; l, \hat{a})\|_q | l \in L \}$$

with L being a set of feasible solutions; options: $q=2$ and $L \subset \mathbb{R}_k$; $q=\infty$ and $L \subset \mathbb{R}^k$; $q=2$ and $L \subset \mathbb{R}_+^k$; $q=\infty$ and $L \subset \mathbb{R}_+^k$.

According to the method set out above, the data are pre-processed. The pre-processing is performed according to known techniques and for known purposes with relation to the methods selected for augmenting resolution of the spectral data and the sensor with which the pre-processing is used. Optionally, one of the following methods is used for normalization of data:

- a) the linear or nonlinear transformation of the λ -axis, aimed at diminishing the non-stationarity effects in the data;
- b) the linear or nonlinear transformation of the y -axis, aimed at diminishing the non-linearity effects in the data;
- c) the linear or nonlinear transformation of the λ -axis and y -axis, aimed at diminishing the non-stationary and non-linearity effects in the data.

Optionally, one of the following methods may be used for smoothing the data:

- a) the linear, FIR-type or IIR-type, filtering;
- b) the median filtering;
- c) the smoothing approximation by cubic splines;
- d) the deconvolution with respect to an identity operator.

Baseline correction is performed according to standard known techniques such as those described in Brame E. G., Grasselli J., *Infrared and Raman Spectroscopy*, Marcel Dekker 1976.

Though the method of augmenting resolution and accuracy of a spectrum from a low resolution captured spectrum according to the invention is described with reference to any hardware implementation of this method, it is preferred that the method is implemented in an integrated hardware device as described herein.

Referring to FIG. 17, a summary of potential applications of the IISS/T in various fields of application is presented. The IISS/T (in the center of the figure) is applied using different spectrometric techniques, which are used in ana-